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     (FILE 'HOME' ENTERED AT 08:31:14 ON 05 SEP 2003)
     FILE 'CA' ENTERED AT 08:31:26 ON 05 SEP 2003
                E NEXPERT
L1            12 S E3
L2             2 S L1 AND MIX?
                E YOSHIKAWA H/AU
L3          2212 S YOSHIKAWA H?/AU
L4          2018 S UENO H?/AU
L5             2 S L3 AND L4
L6           377 S EXPERT AND MIX?
L7            41 S L6 AND(SAFETY OR FLAMMA? OR IMFLAM? OR INFLAM? OR IGNIT?)
L8             2 S L6 AND SPREADSHEET
L9            54 S L6 AND GAS
L10           88 S L2,L7-9
L11          289 S L6 NOT L10
L12           52 S L11 AND PREDICT?

=> d l10 bib,ab 1-88
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L10 ANSWER 26 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 130:269491 CA
TI Optimized kinetics mechanism and calculator for natural **gas** combustion, NOx production and reburning (GRI-MECH 3.0)
AU Frenklach, M.; Goldenberg, M.; Moriarty, N.; Bowman, C. T.; Hanson, R. K.; Davidson, D. F.; Gardiner, W. C., Jr.; Lissianski, V.; Smith, G. P.; Golden, D. M.; Serauskas, R. V.
CS University of California, Berkeley, USA
SO Proceedings of the International Gas Research Conference (1998), (Vol. 5), 329-336
AB A reliable description of natural **gas** oxidn. chem. and assocd. pollutant formation is essential to successful combustion computer modeling, as an aid in improving the design of natural **gas** fired equipment. The chem. reaction mechanism must be faithful to current exptl. and theor. knowledge of the elementary reaction rates involved, successfully account for basic flame properties, **ignition** limits and delays, and be readily available to the natural **gas** combustion research community in a form that can be put to practical use by engineers without chem. kinetics expertise. We describe GRI-Mech 3.0, the most recent version of an optimized kinetics mechanism for natural **gas** oxidn. and NO formation and reburning. A new version of the interactive GRI-Mech Calculator (Version 3.0) allows non-**experts** to represent and solve natural **gas** combustion problems as combinations of well-**mixed** and plug flow reactors.

L10 ANSWER 36 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 127:333276 CA
TI **Spreadsheet** version of knowledge-based system for **mixing** tanks selection
AU Koiranen, Tuomas; Kraslawski, Andrzej; Nystrom, Lars
CS Dep. Chem. Technol., Lappeenranta Univ. Technol., Lappeenranta, SF-53851, Finland
SO Chemical Engineering Communications (1997), 161, 185-204
AB A **spreadsheet**-based **expert** system for the selection of stirred tank vessels is presented. The presented system was designed to work in the narrow field of expertize. The general methodol. of the **mixers** selection is presented first. The program structure and the implementation aspects are discussed further. The last part of the paper presents the example of the system application, comments about the obtained solns. and summary. The **expert**

systems implemented in **spreadsheet** programs are not very popular and there is a common believe that their capabilities are strongly limited. However, this type of **expert** system could be very useful in the equipment selection. The development of the **expert** systems is recommended starting from the specialized tools and next transfer of the structured knowledge systems into **spreadsheet** programs.

L10 ANSWER 47 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 123:147477 CA
TI Knowledge-Based System for the Preliminary Design of **Mixing** Equipment
AU Koiranen, Tuomas; Kraslawski, Andrzej; Nystrom, Lars
CS Department of Chemical Technology, Lappeenranta University of Technology, Lappeenranta, FIN-53851, Finland
SO Industrial & Engineering Chemistry Research (1995), 34(9), 3059-67
AB A methodol. is presented of **mixing** system design and an expert system that is built according to the proposed principles. The knowledge-based system for the predesign of stirred vessels is strongly user-oriented. The presented program selects and designs impeller, tank, and auxiliary equipment (baffles, entering). There are performed **mixing** power and mech. calcns., too. The system is constructed as an object-oriented database in MS-Windows environment. The Excel tables are used, as the databases, for the selection of stirred vessel components. The stirred vessel components are objects in **Nexpert** Object (by Neuron Data Inc.) knowledge bases. A user interface is developed with ToolBook (by Asymetrix Inc). The knowledge bases are activated from the user interface to get the possible selection candidates in ranked order for the problems under consideration. Part of the user interface is an explanation system. The main features of the system are flexibility and good imitation of the design activity.

L10 ANSWER 56 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 119:253067 CA
TI Object-oriented knowledge based systems for process equipment selection
AU Yang, J.; Koiranen, T.; Kraslawski, A.; Nystrom, L.
CS Dep. Chem. Technol., Lappeenranta Univ. Technol., 53851, Finland
SO Computers & Chemical Engineering (1993), 17(12), 1181-9
AB Two prototype knowledge-based systems for shell-and-tube heat exchanger and liq. **mixing** equipment selection (HESES and **MIXES**) are developed by use of **NEXPERT** OBJECT and TOOLBOOK on a PC computer. In the whole system developing procedure the object-oriented approach was used and the object matrix method was proposed to make knowledge acquisition and programming more reasonable, flexible and easier. The object matrixes are stored in MS EXCEL **spreadsheet** files that constitute a primary **expert** interface for knowledge modification. The knowledge bases are organized by a multi-knowledge based technique and the message is transferred among them through a blackboard.

L10 ANSWER 63 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 116:105222 CA
TI CHEMSAFE - a database for **safety** characteristic data
AU Molnarne, M.
CS Bundesanst. Materialforsch. -pruef., Berlin, D-1000/45, Germany
SO Software Dev. Chem. 5, Proc. Workshop "Comput. Chem.", 5th (1991), 45-8. Editor(s): Gmehling, Juergen. Publisher: Springer, Berlin, Germany.
AB CHEMSAFE is a factual database for **flammable** substances. The database consists of rated information about **safety** characteristics of pure compds. and **mixts.** of **gases**, liqs., dusts. The crit. evaluation is carried out by the **experts** of two federal institutions of Germany. The database is available for online recherche at the INKADAT host through FIZ Chemie or can

be installed as inhouse version. subjected to a new trial.

L10 ANSWER 69 OF 88 CA COPYRIGHT 2003 ACS on STN
AN 107:25683 CA
TI Thermodynamics of petroleum **mixtures** containing heavy hydrocarbons: an **expert** tuning system
AU Gani, Rafigul; Fredenslund, Aage
CS Inst. Kemitek., Danmarks Tek. Hojskole, Lyngby, 2800, Den.
SO Industrial & Engineering Chemistry Research (1987), 26(7), 1304-12
AB In the prediction of equation of state models, knowing the sensitivity type of petroleum **mixts**. and the prediction problem type, a tuning policy 1st decides if tuning is possible. If so, it selects a set of candidate adjustable variables. The adjustable variables may be the pure-component hydrocarbon fraction properties, or they may be the binary interaction parameters. Depending on the no. of exptl. data points available, a subset of the candidate adjustable variables is tuned to satisfy the necessary requirements. The applicability of the proposed tuning policy is demonstrated for several petroleum **mixts**. for 24 results with a std. deviation of 9.03 mg/kg.

=> d l12 bib,ab 1-52

L12 ANSWER 25 OF 52 CA COPYRIGHT 2003 ACS on STN
AN 126:147710 CA
TI **Expert** system for **predicting** hazardous conditions of chemical process
AU An, Dae Myung; Hwang, Kyu Suk
CS Dept. of Chem. Eng., Pusan National University, Pusan, 609-735, S. Korea
SO Hwahak Konghak (1996), 34(6), 727-734
LA Korean
AB An **expert** system was developed to **predict** hazardous conditions in chem. plants as an operation-aid system for the automation of unsteady state process operation such as start-up and shutdown. Hazards were classified into 3 main groups; constraints for preoperation and main operation of process units, hazards by **mixing** of dangerous materials, and potential hazards in process. Using these 3 groups, hazardous-condition-database was organized, after that, the methodol. to represent process topol. and process states was developed. An inference engine was developed for evaluating hazards in process and applied to the practical chem. plant to identify various types of hazards.

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STN INTERNATIONAL LOGOFF AT 08:49:45 ON 05 SEP 2003

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(FILE 'HOME' ENTERED AT 09:35:11 ON 05 SEP 2003)
FILE 'CA' ENTERED AT 09:35:21 ON 05 SEP 2003
E ILLY F/AU
L1 6 S E3-4
L2 2 S L1 AND REACTIVE
L3 6107 S REACT?(2A)(GAS OR VAPOR OR VOLATILE)(10A)(MIX? OR COMBIN?)
L4 105 S L3 AND(RISK? OR HAZA? OR SAFE?)
L5 9 S L4 AND(COMPUTER OR OPTIMI?)

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STN INTERNATIONAL LOGOFF AT 09:47:13 ON 05 SEP 2003